



# **STIC Search Report**

## **Biotech-Chem Library**

**STIC Database Tracking Number: 153470**

**TO: Rei-Tsang Shiao**  
**Location: 5a10 / 5c18**  
**Monday, May 16, 2005**  
**Art Unit: 1626**  
**Phone: 571-272-0707**  
**Serial Number: 10 / 659193**

**From: Jan Delaval**  
**Location: Biotech-Chem Library**  
**Remsen 1a51**  
**Phone: 571-272-2504**  
**jan.delaval@uspto.gov**

### **Search Notes**

Jan Pelam  
for search

Access DB# 153470

# SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Robert (Raj) Shah Examiner #: 79521 Date: 5/6/05  
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/659,193  
Mail Box and Bldg/Room Location: 5A10/5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

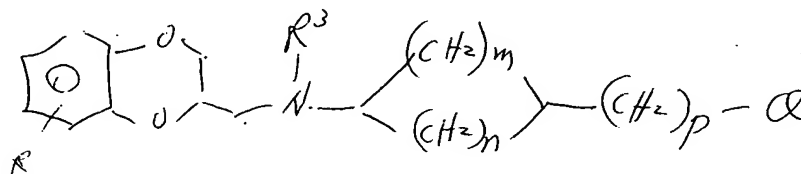
Title of invention: Anti-depressant cycloalkylamine derivatives

Inventors (please provide full names): Ervin et al

Earliest Priority Filing Date: \_\_\_\_\_

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

I. Search opaz



\* 1. Q is sub. ie. aryl, heteroaryl, heterocycle

2. R<sup>3</sup> is sub

3. m, n is 1~3. p is 0 to 3.

II. methods of use of opaz.

## STAFF USE ONLY

Searcher: Jan  
Searcher Phone #: 22504  
Searcher Location: \_\_\_\_\_  
Date Searcher Picked Up: 5/16/05  
Date Completed: 5/16/05  
Searcher Pre-Review Time: \_\_\_\_\_  
Critical Prep Time: 1.5  
Time: 7:10

## Type of Search

NA Sequence (#) \_\_\_\_\_  
AA Sequence (#) \_\_\_\_\_  
Structure (#) ✓  
Bibliographic \_\_\_\_\_  
Litigation \_\_\_\_\_  
Fulltext \_\_\_\_\_  
Patent Family \_\_\_\_\_  
Other \_\_\_\_\_

## Vendors and cost where applicable

STN ✓  
Dialog \_\_\_\_\_  
Questel/Orbit \_\_\_\_\_  
Dr. Link \_\_\_\_\_  
Lexis/Nexis \_\_\_\_\_  
Sequence Systems \_\_\_\_\_  
WWW/Internet \_\_\_\_\_  
Other (Specify) \_\_\_\_\_

=> fil reg

FILE 'REGISTRY' ENTERED AT 13:48:53 ON 16 MAY 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2005 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 MAY 2005 HIGHEST RN 850445-20-4

DICTIONARY FILE UPDATES: 15 MAY 2005 HIGHEST RN 850445-20-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

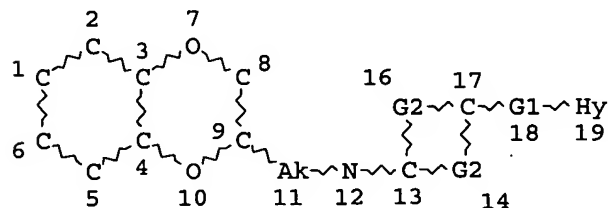
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*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
*****
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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l14

L8 STR



REP G1=(0-1) AK

REP G2=(1-3) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

L10 92 SEA FILE=REGISTRY SSS FUL L8

L11 44 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND (NC4-C6 OR OC4-C6 OR SC4-C6)/ES

L12 44 SEA FILE=REGISTRY ABB=ON PLU=ON L11 AND (C4 OR C5 OR C6 OR C7 OR C8)/ES

L13 26 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT OC2OC2-C6/ES  
L14 18 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT L13

=> d his

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SET COST OFF

FILE 'HCAPLUS' ENTERED AT 13:40:30 ON 16 MAY 2005

L1 1 S US20040127543/PN OR (US2003-659193# OR WO2003-US28296 OR US20  
E EVRARD D/AU  
L2 42 S E3,E4,E8-E10  
E SHAH U/AU  
E URESH/AU  
E SHANTILAL/AU  
E STACK G/AU  
L3 101 S E3,E6,E11,E12  
E SHAH U/AU  
L4 40 S E3,E6,E22-E24  
E WYETH/PA,CS  
L5 4356 S E3,E4 OR WYETH?/PA,CS  
SEL RN L1

FILE 'REGISTRY' ENTERED AT 13:43:17 ON 16 MAY 2005

L6 36 S E1-E36  
L7 16 S L6 AND NR>=5  
L8 STR  
L9 0 S L8  
L10 92 S L8 FUL  
SAV L10 SHIAO659/A  
L11 44 S L10 AND (NC4-C6 OR OC4-C6 OR SC4-C6)/ES  
L12 44 S L11 AND (C4 OR C5 OR C6 OR C7 OR C8)/ES  
L13 26 S L12 NOT OC2OC2-C6/ES  
L14 18 S L12 NOT L13  
L15 2 S L14 NOT L7  
L16 18 S L7,L14,L15  
SAV L16 SHIAO659A/A  
L17 74 S L10 NOT L16

FILE 'HCAOLD' ENTERED AT 13:48:11 ON 16 MAY 2005

L18 0 S L16

FILE 'HCAPLUS' ENTERED AT 13:48:14 ON 16 MAY 2005

L19 2 S L16  
L20 2 S L19 AND L1-L5

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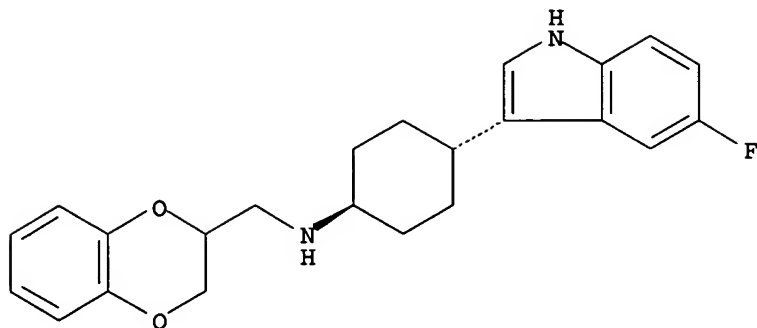
L21 1 S L16

FILE 'REGISTRY' ENTERED AT 13:48:53 ON 16 MAY 2005

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L16 ANSWER 1 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 848072-03-7 REGISTRY  
ED Entered STN: 07 Apr 2005  
CN 1,4-Benzodioxin-2-methanamine, N-[trans-4-(5-fluoro-1H-indol-3-yl)cyclohexyl]-2,3-dihydro- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H25 F N2 O2  
SR CA  
LC STN Files: CA, CAPLUS

Relative stereochemistry.



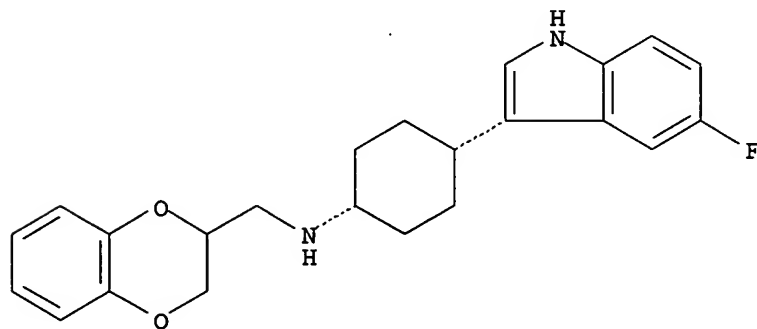
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:309195

L16 ANSWER 2 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 848072-02-6 REGISTRY  
ED Entered STN: 07 Apr 2005  
CN 1,4-Benzodioxin-2-methanamine, N-[cis-4-(5-fluoro-1H-indol-3-yl)cyclohexyl]-2,3-dihydro- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H25 F N2 O2  
SR CA  
LC STN Files: CA, CAPLUS

Relative stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

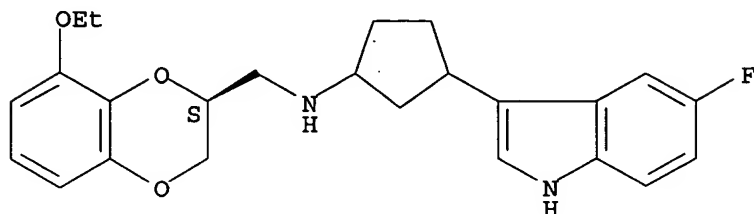
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 142:309195

L16 ANSWER 3 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-76-2 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-

yl)cyclopentyl]-2,3-dihydro-, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H27 F N2 O3  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



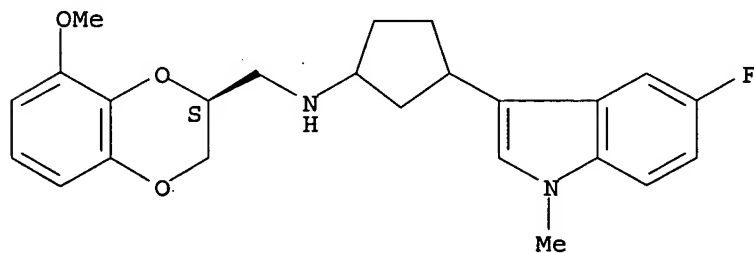
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 4 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-75-1 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H27 F N2 O3  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

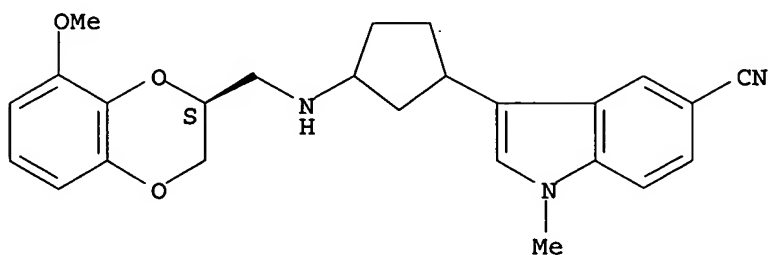
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L16 ANSWER 5 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-60-4 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-

benzodioxin-2-yl)methyl]amino]cyclopentyl]-1-methyl-, monohydrochloride  
(9CI) (CA INDEX NAME)

FS STEREOSEARCH  
MF C25 H27 N3 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (675831-59-1)

Absolute stereochemistry.



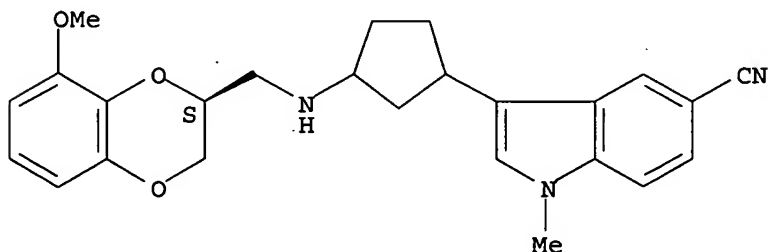
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 6 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-59-1 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl)methyl]amino]cyclopentyl]-1-methyl- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C25 H27 N3 O3  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



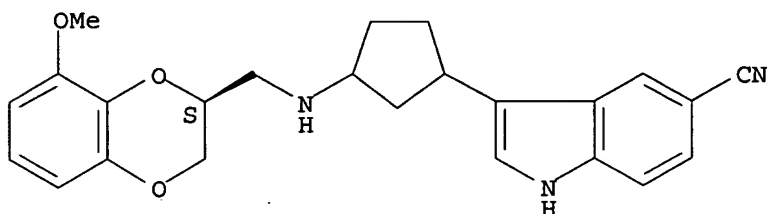
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REFERENCE 1: 140:287394

L16 ANSWER 7 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-58-0 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]-, monohydrochloride (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H25 N3 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (675831-57-9)

Absolute stereochemistry.



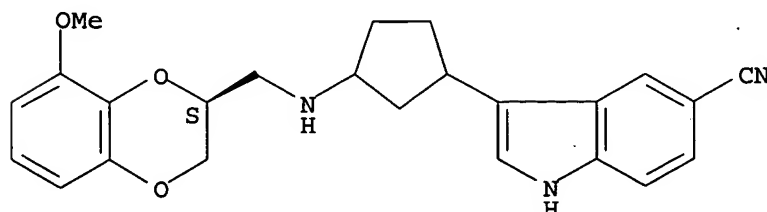
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 8 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-57-9 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H25 N3 O3  
CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

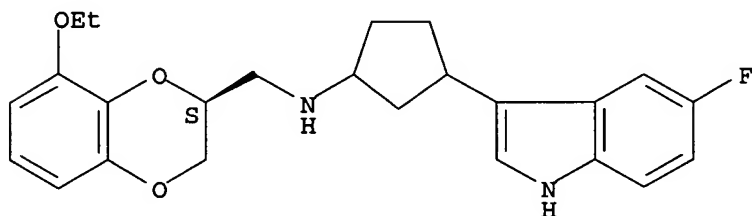
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394



L16 ANSWER 9 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-56-8 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H27 F N2 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (675831-76-2)

Absolute stereochemistry.



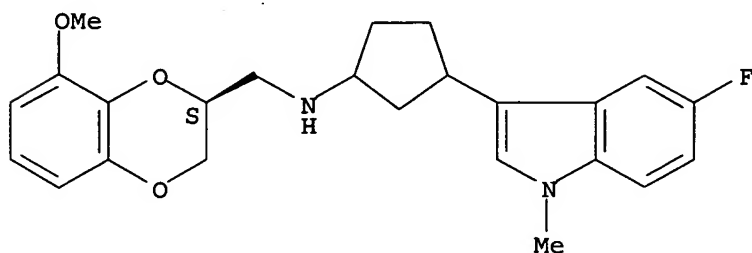
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1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 10 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-55-7 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C24 H27 F N2 O3 . Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (675831-75-1)

Absolute stereochemistry.



● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

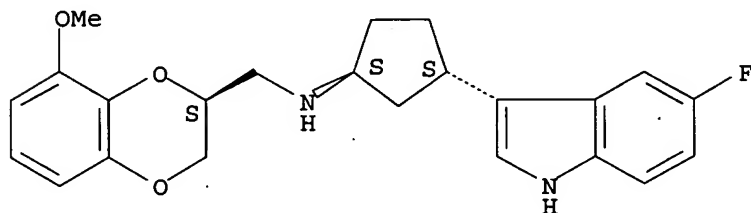
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CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)-, (2E)-2-butenedioate (9CI)  
(CA INDEX NAME)  
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MF C23 H25 F N2 O3 . x C4 H4 O4  
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LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

CM 1

CRN 675831-52-4  
CMF C23 H25 F N2 O3

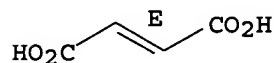
Absolute stereochemistry.



CM 2

CRN 110-17-8  
CMF C4 H4 O4

Double bond geometry as shown.

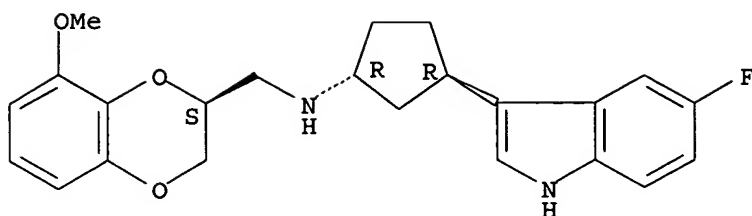


1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 12 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-53-5 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H25 F N2 O3 . x Cl H  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL  
CRN (675831-51-3)

Absolute stereochemistry. Rotation (-).



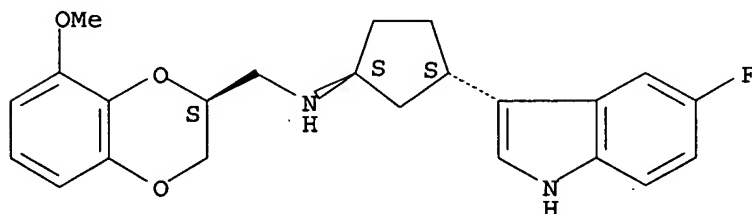
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REFERENCE 1: 140:287394

L16 ANSWER 13 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-52-4 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)-(9CI) (CA INDEX NAME)  
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SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.



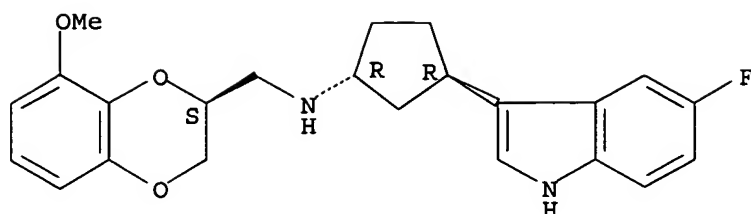
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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RN 675831-51-3 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)-(9CI) (CA INDEX NAME)  
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SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).



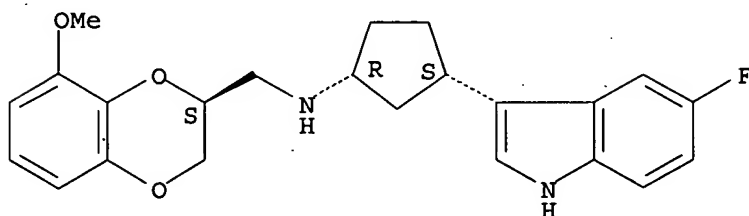
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 15 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-50-2 REGISTRY  
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(CA INDEX NAME)  
FS STEREOSEARCH  
MF C23 H25 F N2 O3 . Cl H  
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Absolute stereochemistry. Rotation (-).



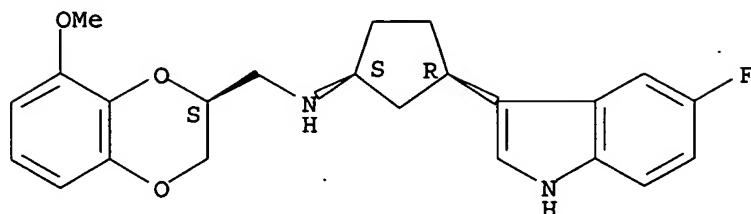
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MF C23 H25 F N2 O3 . Cl H  
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Absolute stereochemistry. Rotation (-).



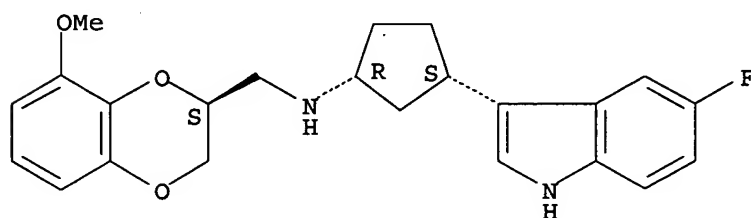
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1 REFERENCES IN FILE CA (1907 TO DATE)  
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REFERENCE 1: 140:287394

L16 ANSWER 17 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-48-8 REGISTRY  
ED Entered STN: 16 Apr 2004  
CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)  
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Absolute stereochemistry. Rotation (-).



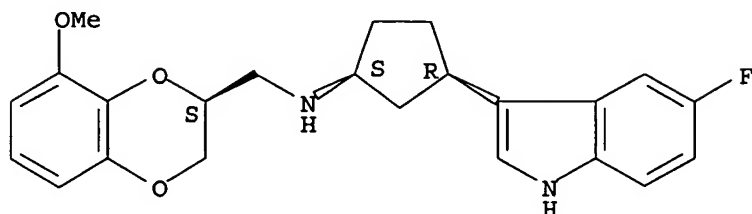
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

L16 ANSWER 18 OF 18 REGISTRY COPYRIGHT 2005 ACS on STN  
RN 675831-47-7 REGISTRY  
ED Entered STN: 16 Apr 2004  
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FS STEREOSEARCH  
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CI COM  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (-).



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 140:287394

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FILE 'USPAT2' ENTERED AT 13:49:57 ON 16 MAY 2005  
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=> d/bib abs hitstr

L21 ANSWER 1 OF 1. USPATFULL on STN

AN 2004:166053 USPATFULL

TI Antidepressant cycloalkylamine derivatives of 2,3-dihydro-1,4-benzodioxan

IN Evrard, Deborah Ann, Hamilton Square, NJ, UNITED STATES  
Shah, Uresh Shantilal, Cranbury, NJ, UNITED STATES  
Stack, Gary Paul, Ambler, PA, UNITED STATES

PI US 2004127543 A1 20040701

AI US 2003-659193 A1 20030910 (10)

PRAI US 2002-410169P 20020912 (60)

DT Utility

FS APPLICATION

LREP WOODCOCK WASHBURN LLP, ONE LIBERTY PLACE, 46TH FLOOR, 1650 MARKET STREET, PHILADELPHIA, PA, 19103

CLMN Number of Claims: 31

ECL Exemplary Claim: 1

DRWN No Drawings

LN.CNT 920

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB Compounds of the Formula I: ##STR1##

are useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as pre-menstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alcohol addiction, sexual dysfunction and related illnesses.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

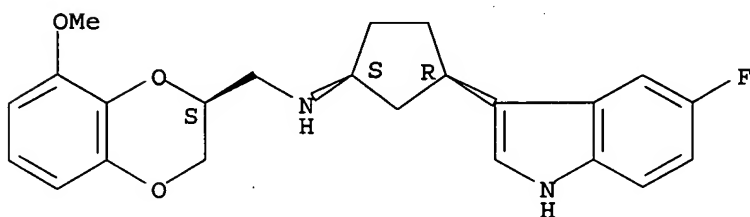
IT 675831-47-7P 675831-48-8P 675831-49-9P  
 675831-50-2P 675831-51-3P 675831-52-4P  
 675831-53-5P 675831-54-6P 675831-55-7P  
 675831-56-8P 675831-57-9P 675831-58-0P  
 675831-59-1P 675831-60-4P 675831-75-1P  
 675831-76-2P

(preparation of antidepressant cycloalkylamine derivs. of  
 2,3-dihydro-1,4-benzodioxane)

RN 675831-47-7 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

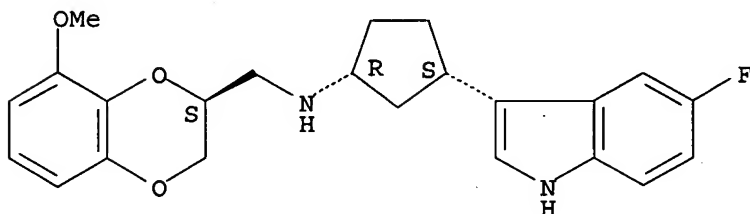
Absolute stereochemistry. Rotation (-).



RN 675831-48-8 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

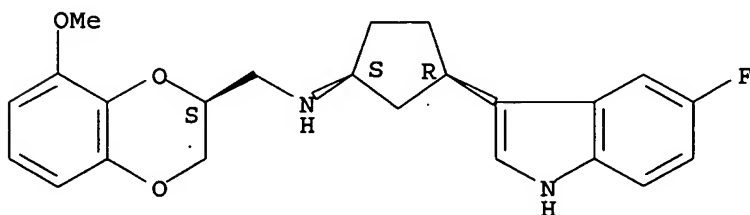
Absolute stereochemistry. Rotation (-).



RN 675831-49-9 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



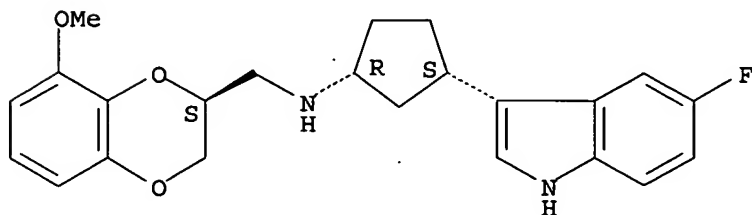
● HCl

RN 675831-50-2 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3S)-3-(5-fluoro-1H-indol-3-

yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

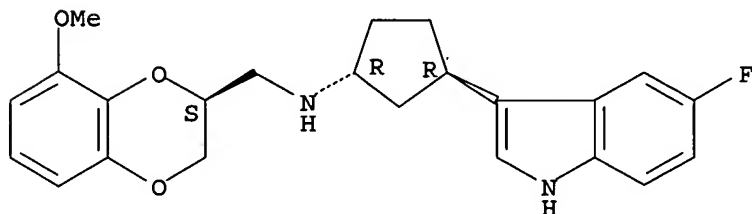


● HCl

RN 675831-51-3 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

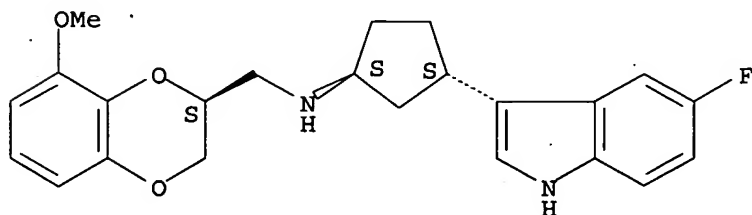
Absolute stereochemistry. Rotation (-).



RN 675831-52-4 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

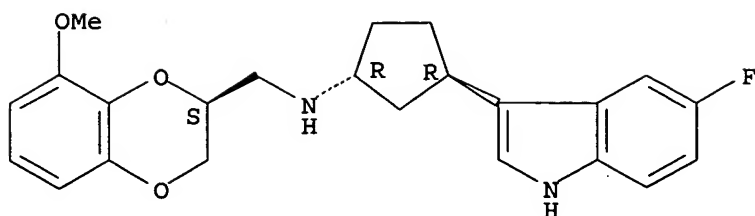


RN 675831-53-5 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).





● x HCl

RN 675831-54-6 USPATFULL

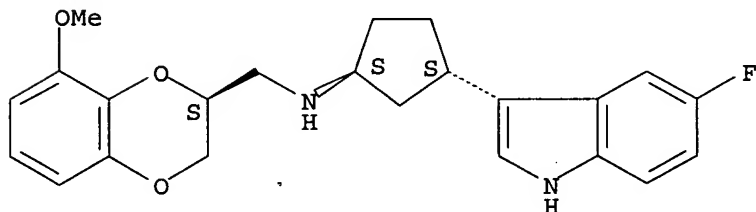
CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)-, (2E)-2-butenedioate (9CI)  
(CA INDEX NAME)

CM 1

CRN 675831-52-4

CMF C23 H25 F N2 O3

Absolute stereochemistry.



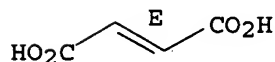
CM 2

CRN 110-17-8

CMF C4 H4 O4

CDES 2:E

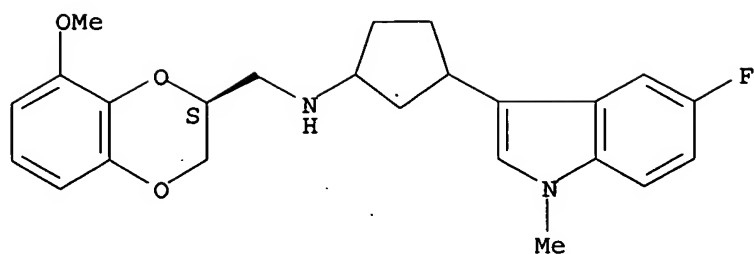
Double bond geometry as shown.



RN 675831-55-7 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

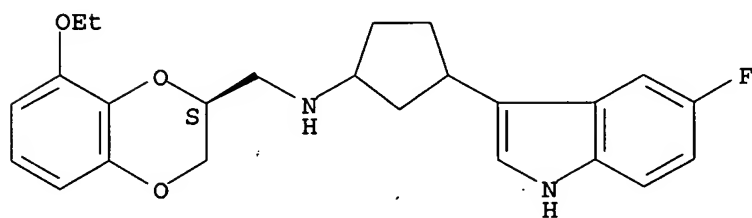


● HCl

RN 675831-56-8 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

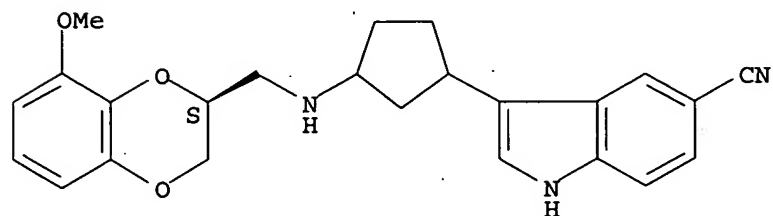


● HCl

RN 675831-57-9 USPATFULL

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]- (9CI) (CA INDEX NAME)

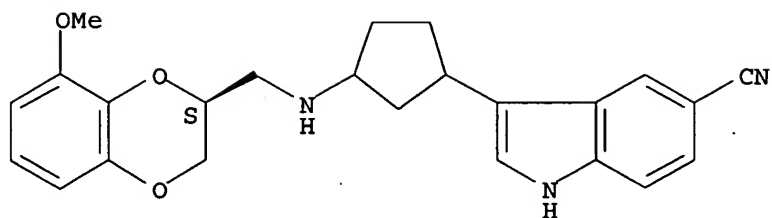
Absolute stereochemistry.



RN 675831-58-0 USPATFULL

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

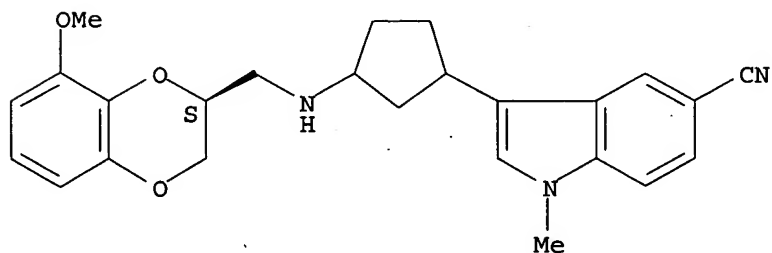


● HCl

RN 675831-59-1 USPATFULL

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]-1-methyl- (9CI) (CA INDEX NAME)

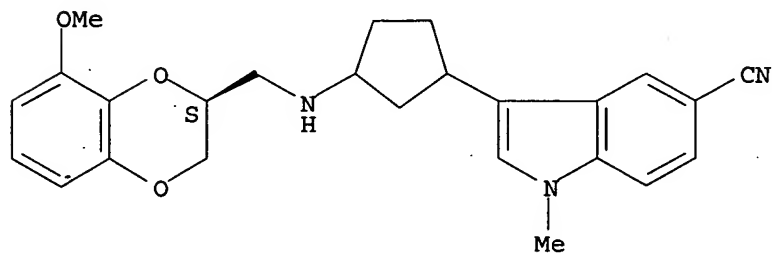
Absolute stereochemistry.



RN 675831-60-4 USPATFULL

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

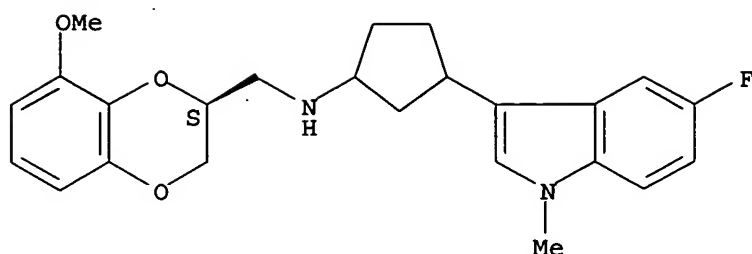


● HCl

RN 675831-75-1 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

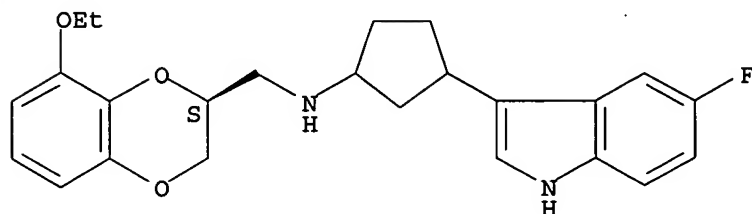
Absolute stereochemistry.



RN 675831-76-2 USPATFULL

CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> fil hcaplus

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L20 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:86370 HCAPLUS

DN 142:309195

ED Entered STN: 01 Feb 2005

TI Studies towards the next generation of antidepressants. Part 4: Derivatives of 4-(5-fluoro-1H-indol-3-yl)cyclohexylamine with affinity for

the serotonin transporter and the 5-HT1A receptor

AU **Evrard, Deborah A.**; Zhou, Ping; Yi, Soo Y.; Zhou, Dahui; Smith, Deborah L.; Sullivan, Kelly M.; Hornby, Geoffrey A.; Schechter, Lee E.; Andree, Terrance H.; Mewshaw, Richard E.

CS Chemical and Screening Sciences, **Wyeth Research**, Princeton, NJ, 08543, USA

SO Bioorganic & Medicinal Chemistry Letters (2005), 15(4), 911-914  
CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier B.V.

DT Journal

LA English

CC 1-3 (Pharmacology)  
Section cross-reference(s): 28

AB Derivs. of the serotonin reuptake inhibitor 4-(5-fluoro-1H-indol-3-yl)cyclohexylamine, in which serotonin 1A (5-HT1A) receptor pharmacophoric elements are incorporated, are reported. Analogs exhibiting affinity for both the serotonin transporter and the 5-HT1A receptor are described. Compds. containing 1-(4-indolyl)piperazine and 2-(1H-indol-4-yloxy)ethylamine are promising leads for further SAR studies.

ST fluorindolyl cyclohexylamine prepn antidepressant serotonin transporter SAR

IT 246027-95-2P 246027-97-4P 246028-03-5P 246028-05-7P 246028-11-5P  
246028-14-8P 282543-73-1P 282543-75-3P 282544-29-0P 282544-48-3P  
282544-50-7P 848072-01-5P **848072-02-6P 848072-03-7P**  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(Studies towards the next generation of antidepressants, derivs. of cyclohexylamine with affinity for the serotonin transporter)

IT 100-46-9, Benzylamine, reactions 631-61-8, Ammonium acetate 1094-91-3, 2-Tosyloxymethyl-1,4-benzodioxane 1836-62-0 32604-73-2 35386-24-4  
84807-09-0 98224-03-4 185383-64-6 246028-97-7  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(Studies towards the next generation of antidepressants, derivs. of cyclohexylamine with affinity for the serotonin transporter)

IT 246029-23-2P 246029-24-3P 369365-50-4P 675879-60-4P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(Studies towards the next generation of antidepressants, derivs. of cyclohexylamine with affinity for the serotonin transporter)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT 848072-02-6P 848072-03-7P

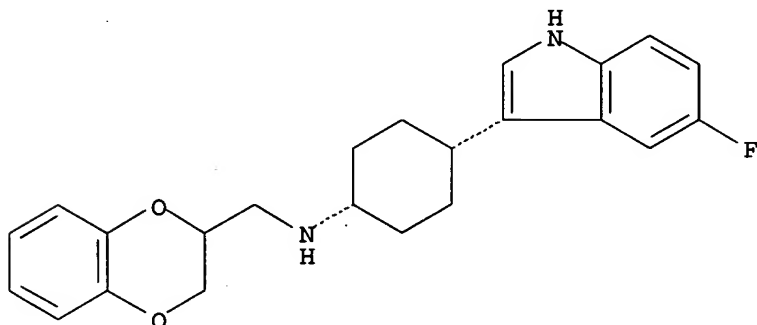
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(Studies towards the next generation of antidepressants, derivs. of cyclohexylamine with affinity for the serotonin transporter)

RN 848072-02-6 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[cis-4-(5-fluoro-1H-indol-3-yl)cyclohexyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

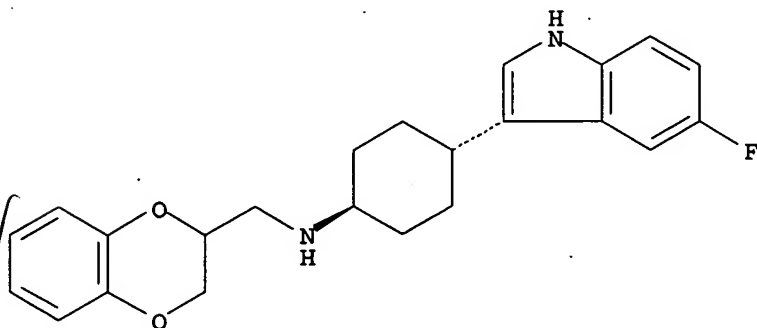
Relative stereochemistry.



RN 848072-03-7 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[trans-4-(5-fluoro-1H-indol-3-yl)cyclohexyl]-2,3-dihydro- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:252509 HCAPLUS

DN 140:287394

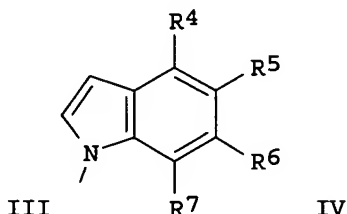
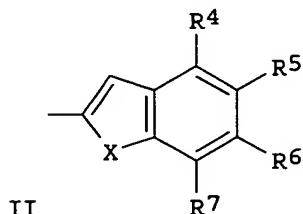
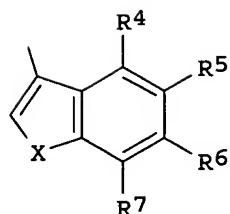
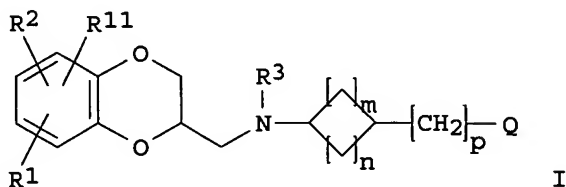
ED Entered STN: 26 Mar 2004

TI Preparation of antidepressant cycloalkylamine derivatives of  
 2,3-dihydro-1,4-benzodioxane  
 IN Evrard, Deborah Ann; Shah, Uresh Shantilal;  
 Stack, Gary Paul  
 PA Wyeth, John, and Brother Ltd., USA  
 SO PCT Int. Appl., 39 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D405-12  
 ICS A61K031-40; A61P025-24  
 CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 63  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 2004024723	A1	20040325	WO 2003-US28296	20030911 <--	
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	RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG		
	US 2004127543	A1	20040701	US 2003-659193	20030910 <--	
PRAI	US 2002-410169P	P	20020912 <--			

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004024723	ICM	C07D405-12
	ICS	A61K031-40; A61P025-24
US 2004127543	NCL	514/414.000; 514/443.000; 514/452.000; 548/454.000; 549/049.000; 549/358.000
	ECLA	C07D405/12+319+209C <--
OS	MARPAT 140:287394	
GI		



- AB The title compds. [I; R11, R1, R2 = H, halo, CN, carboxamido, etc.; R3 = H, alkyl; m = 1-3; n = 1-2; p = 0-3 (with the proviso that when p = 0, both m and n may not be 2); Q = II-IV (R4-R7 = H, halo, CN, etc.; X = NR8, O, S; R8 = H, alkyl)], useful for the treatment of depression (including but not limited to major depressive disorder, childhood depression and dysthymia), anxiety, panic disorder, post-traumatic stress disorder, premenstrual dysphoric disorder (also known as premenstrual syndrome), attention deficit disorder (with and without hyperactivity), obsessive compulsive disorder, social anxiety disorder, generalized anxiety disorder, obesity, eating disorders such as anorexia nervosa and bulimia nervosa, vasomotor flushing, cocaine and alc. addiction, sexual dysfunction and related illnesses, were prepared Thus, reacting [(2R)-8-methoxy-2,3-dihydro-1,4-benzodioxin-2-yl)methyl 4-methylbenzenesulfonate with cis-3-(5-fluoro-1H-indol-3-yl)cyclopentylamine (preparation given) in DMSO afforded 48% N-[(cis)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-N-{[(2S)-8-methoxy-2,3-dihydro-1,4-benzodioxin-2-yl)methyl}amine. The latter was separated into two diastereoisomers and biol. data (5-HT transporter affinity, 5-HT1A receptor affinity, and antagonistic activity at 5-HT1A receptors were tested) were given for the mixture and both separated isomers. The pharmaceutical composition comprising the compound I is claimed.
- ST antidepressant cycloalkylamine benzodioxane prepn serotonin 5HT1A antagonist; indolylcyclopentylaminomethyl benzodioxane prepn serotonin transporter anxiolytic antiobesity eating disorder; cyclopentylaminomethyl indolyl benzodioxane prepn antidepressant anxiolytic antiobesity eating disorder
- IT 5-HT antagonists  
(5-HT1A; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Appetite  
(anorexia nervosa, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Mental disorder  
(attention deficit disorder, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Appetite  
(bulimia, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Drug dependence  
(cocaine addiction; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Mental disorder  
(depression, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Menopause  
(disorder, hot flash, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Appetite  
Sexual behavior  
(disorder, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Anxiety  
(generalized, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Mental disorder  
(neurotic depression, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Mental disorder  
(obsession-compulsion, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)
- IT Anxiety  
(panic disorder, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)



IT Mental disorder  
(post-traumatic stress disorder, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT Ovarian cycle  
(premenstrual syndrome, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT Antidepressants  
Antiobesity agents  
Anxiolytics  
Appetite depressants  
Human  
(preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT Transport proteins  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(serotonin transporter; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT Anxiety  
(social, treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT Alcoholism  
Anxiety  
Obesity  
(treatment of; preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT 675831-47-7P 675831-48-8P 675831-49-9P  
675831-50-2P 675831-51-3P 675831-52-4P  
675831-53-5P 675831-54-6P 675831-55-7P  
675831-56-8P 675831-57-9P 675831-58-0P  
675831-59-1P 675831-60-4P 675831-75-1P  
675831-76-2P  
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT 100-46-9, Benzylamine, reactions 399-52-0, 5-Fluoroindole 930-30-3,  
2-Cyclopenten-1-one 15861-24-2, 5-Cyanoindole 329966-21-4  
473968-96-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

IT 675831-61-5P 675831-62-6P 675831-63-7P, 3-(5-Fluoro-1H-indol-3-yl)cyclopentanone 675831-64-8P, 3-(3-Oxocyclopentyl)-1H-indole-5-carbonitrile 675831-65-9P, 3-(5-Fluoro-1-methyl-1H-indol-3-yl)cyclopentanone 675831-66-0P, 1-Methyl-3-(3-oxocyclopentyl)-1H-indole-5-carbonitrile 675831-67-1P 675831-68-2P 675831-69-3P 675831-70-6P  
675831-71-7P 675831-72-8P 675831-73-9P 675831-74-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE  
(1) American Home Prod; WO 9951592 A 1999 HCAPLUS  
(2) Cipollina, J; US 5468767 A 1995 HCAPLUS  
(3) Cipollina, J; US 5607961 A 1997 HCAPLUS

IT 675831-47-7P 675831-48-8P 675831-49-9P  
675831-50-2P 675831-51-3P 675831-52-4P  
675831-53-5P 675831-54-6P 675831-55-7P  
675831-56-8P 675831-57-9P 675831-58-0P  
675831-59-1P 675831-60-4P 675831-75-1P  
675831-76-2P

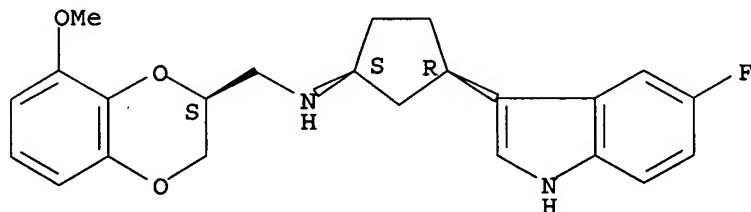
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of antidepressant cycloalkylamine derivs. of 2,3-dihydro-1,4-benzodioxane)

RN 675831-47-7 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

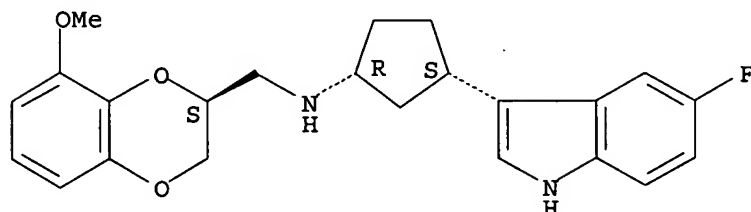
Absolute stereochemistry. Rotation (-).



RN 675831-48-8 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

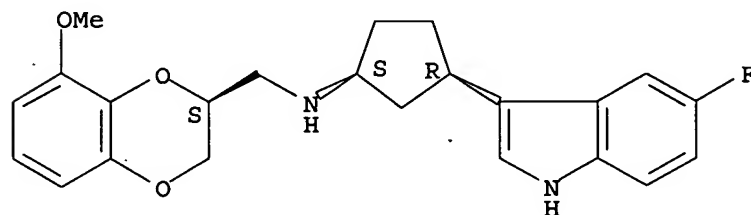
Absolute stereochemistry. Rotation (-).



RN 675831-49-9 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

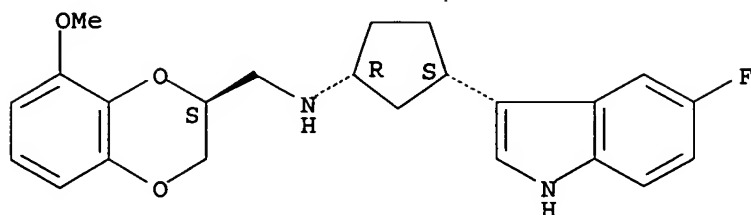


● HCl

RN 675831-50-2 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

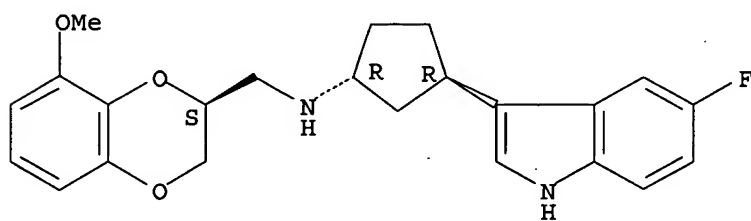


● HCl

RN 675831-51-3 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

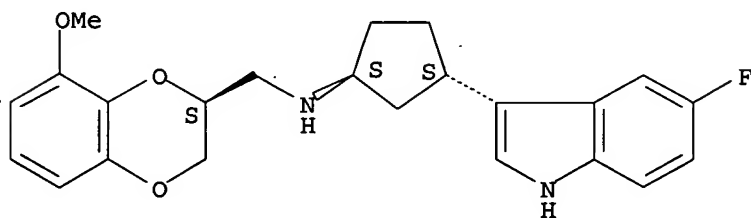
Absolute stereochemistry. Rotation (-).



RN 675831-52-4 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

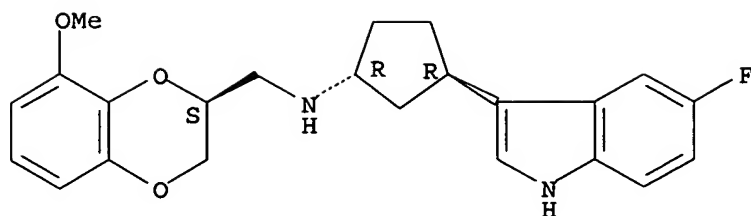
Absolute stereochemistry.



RN 675831-53-5 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[(1R,3R)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, hydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



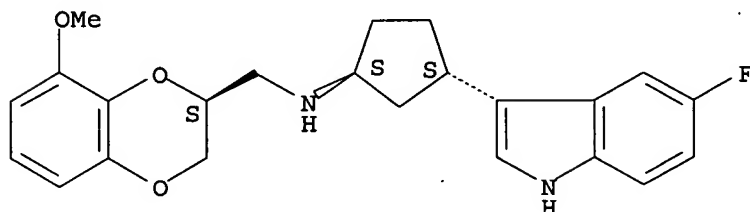
●<sub>x</sub> HCl

RN 675831-54-6 HCAPLUS  
 CN 1,4-Benzodioxin-2-methanamine, N-[(1S,3S)-3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)-, (2E)-2-butenedioate (9CI)  
 (CA INDEX NAME)

CM 1

CRN 675831-52-4  
 CMF C23 H25 F N2 O3

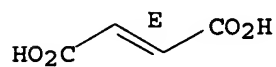
Absolute stereochemistry.



CM 2

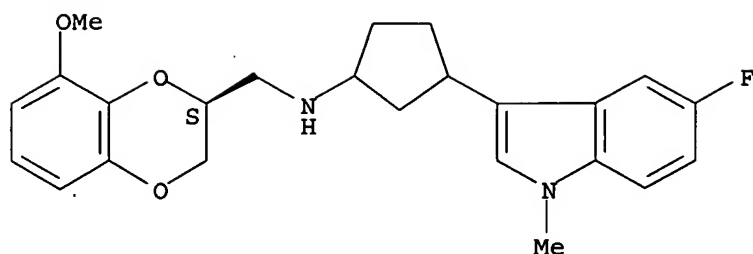
CRN 110-17-8  
 CMF C4 H4 O4

Double bond geometry as shown.



RN 675831-55-7 HCAPLUS  
 CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, monohydrochloride, (2S)- (9CI)  
 (CA INDEX NAME)

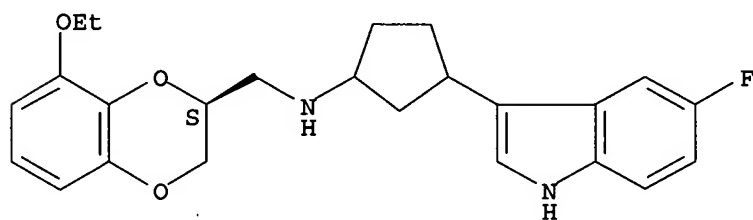
Absolute stereochemistry.



● HCl

RN 675831-56-8 HCAPLUS  
 CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

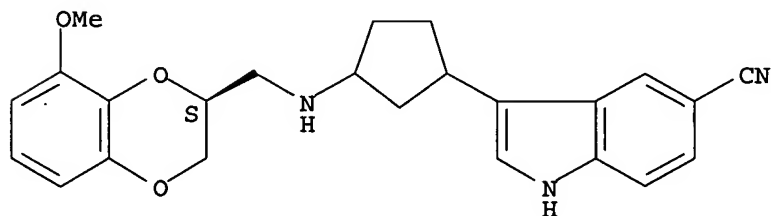
Absolute stereochemistry.



● HCl

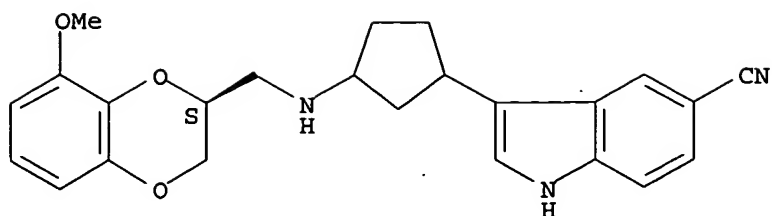
RN 675831-57-9 HCAPLUS  
 CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 675831-58-0 HCAPLUS  
 CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl]methyl]amino]cyclopentyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

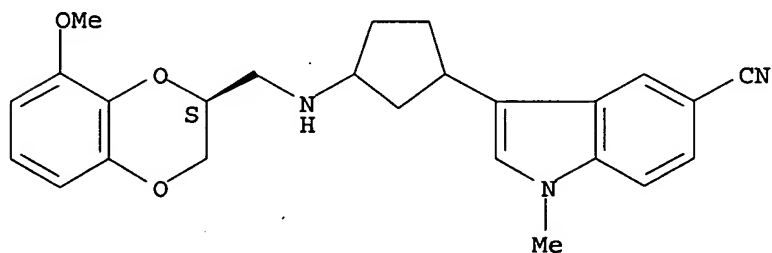


● HCl

RN 675831-59-1 HCAPLUS

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl)methyl]amino]cyclopentyl]-1-methyl- (9CI) (CA INDEX NAME)

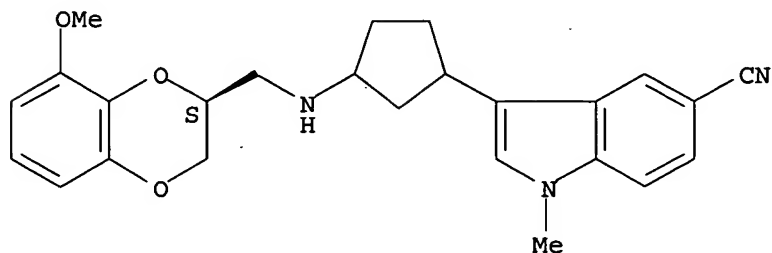
Absolute stereochemistry.



RN 675831-60-4 HCAPLUS

CN 1H-Indole-5-carbonitrile, 3-[3-[[[(2S)-2,3-dihydro-8-methoxy-1,4-benzodioxin-2-yl)methyl]amino]cyclopentyl]-1-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

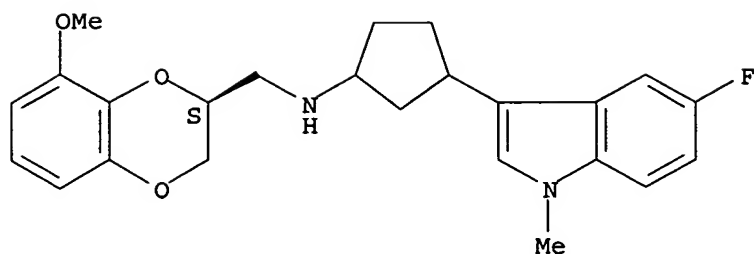


● HCl

RN 675831-75-1 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, N-[3-(5-fluoro-1-methyl-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-8-methoxy-, (2S)- (9CI) (CA INDEX NAME)

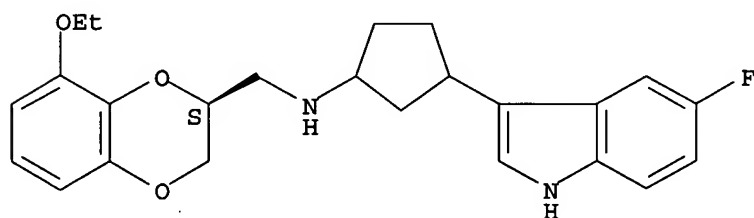
Absolute stereochemistry.



RN 675831-76-2 HCAPLUS

CN 1,4-Benzodioxin-2-methanamine, 8-ethoxy-N-[3-(5-fluoro-1H-indol-3-yl)cyclopentyl]-2,3-dihydro-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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